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Los Alamos National Laboratory

FY18 Science Accomplishments



We see an enduring future for an integrated Laboratory — and the need for integrating assets at scale for national security

NUCLEAR WEAPON MISSION



NUCLEAR GLOBAL SECURITY MISSION

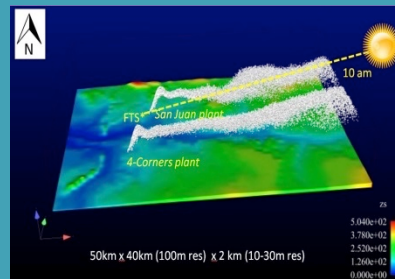


Four capability pillars define key areas of science, technology & engineering in which we must lead



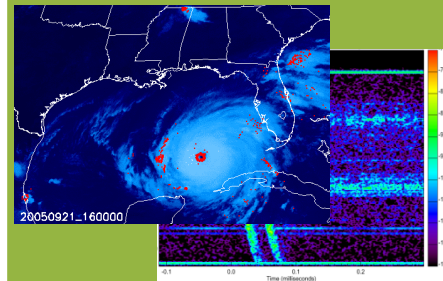
MATERIALS FOR THE FUTURE

Defects and Interfaces
Extreme Environments
Emergent Phenomena



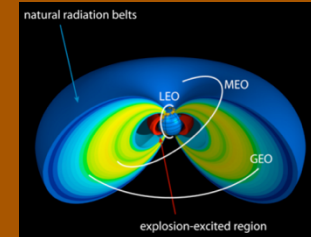
SCIENCE OF SIGNATURES

Discover Signatures
Revolutionize Measurements
Forward Deployment



INTEGRATING INFORMATION, SCIENCE, AND TECHNOLOGY FOR PREDICTION

Complex Networks
Computational Co-Design
Data Science at Scale



NUCLEAR AND PARTICLE FUTURES

High Energy Density Physics & Fluid Dynamics
Nuclear & Particle Physics, Astrophysics & Cosmology
Applied Nuclear Science & Engineering
Accelerators Science & Technology

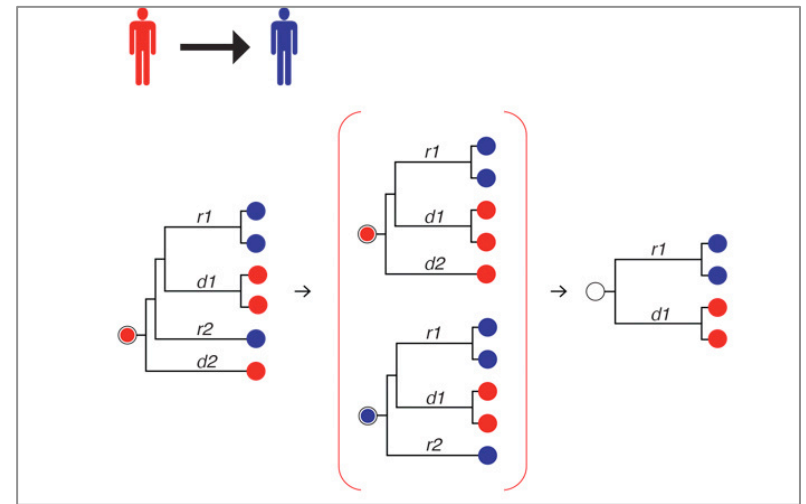
We invest LDRD (6% of budget) to foster capability in support of mission consistent with the pillars

UNCLASSIFIED

July 23, 2018 | 3

LANL computer simulations predict the spread of HIV

- Los Alamos computer simulations accurately traced origin and predicted HIV transmission through populations (*Nature Microbiology* 2018)
- Researchers tracked the paths of HIV's changing genetic patterns to determine an infection's origin and timeframe
 - Simulations were consistent with actual DNA database of more than 840,000 HIV sequences
- The Lab is now collaborating with Colorado & Michigan state health agencies to develop computational tools that will help the agencies track the disease and allocate resources for targeted prevention campaigns

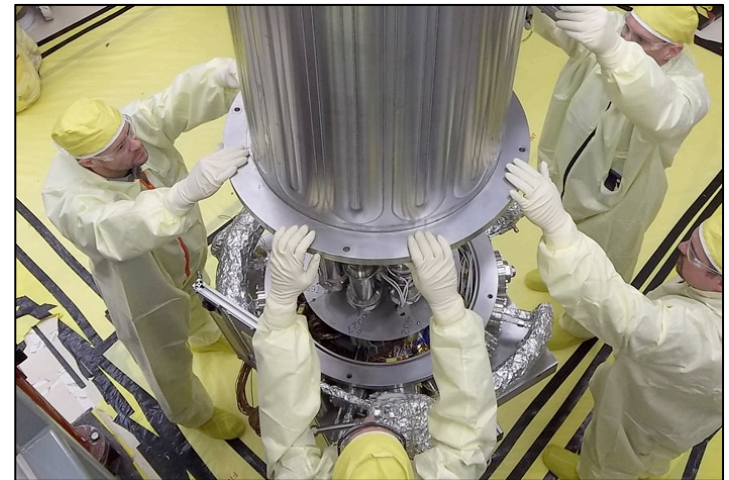


Researchers used phylogenetic methods, examining evolutionary relationships in the virus's genetic code to evaluate its transmission

Cutting-edge modeling tools like this can be used to predict patterns of other rapidly evolving infectious diseases

New, small nuclear power system passes operating tests, demonstrating possible use for space missions

- Kilopower is a small, lightweight fission power system that can provide up to 10 kilowatts of electrical power continuously for at least 10 years
 - Prototype power system uses a solid, cast uranium-235 reactor core; Passive sodium heat pipes transfer reactor heat to high-efficiency Stirling engines
- The KRUSTY (Kilopower Using Stirling Technology) experiment tested the system for five months at NNSA's Nevada National Security Site
 - Throughout the experiment, the team simulated power reduction, failed engines, and failed heat pipes
 - Kilopower reliably creates electricity with fission power and is stable and safe in any environment

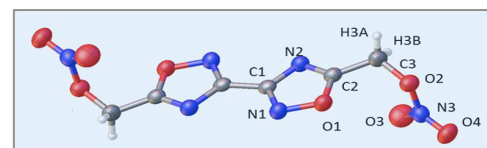


NASA & NNSA engineers lower the wall of the vacuum chamber around the KRUSTY system at the Nevada National Security Site (NNSS).

Based on the successful experiment, the Kilopower system promises to be an essential part of future missions to the Moon, Mars

Scientists develop potential replacement for toxic TNT

- LANL scientists, working with the U.S. Army Research Laboratory, developed a novel “melt-cast” explosive material that could be a suitable replacement for Trinitrotoluene (TNT) (*Organic Process R&D* 2018)



- TNT is listed as a possible carcinogen and is toxic to the environment
 - Challenges included developing an practical and affordable explosive with low or no toxicity, high synthetic yields, and a melting point that allows it to be liquefied and cast
- The new molecule is a nitrogen-containing compound called bis-oxadiazole
 - Has a performance 1.5 times greater than TNT and a lower sensitivity



Los Alamos explosives chemist David Chavez pours an example of melt-castable explosive into a copper mold.

TNT replacement could provide enhanced performance, safety and support additive manufacturing

Levitation of ultracold neutrons at LANSCE linear accelerator yields neutron-lifetime measurement

- In an experiment at the Los Alamos linear accelerator, ultracold neutrons were levitated so their actual lifetimes can be more accurately measured (***Science* 2018**)
- For the first time, the measurements are considered accurate enough that potential corrections are not larger than the uncertainties
- Results stem from 10 years of research between Los Alamos and numerous collaborators
- The study paves the way for a better understanding of how atoms were first created during the Big Bang

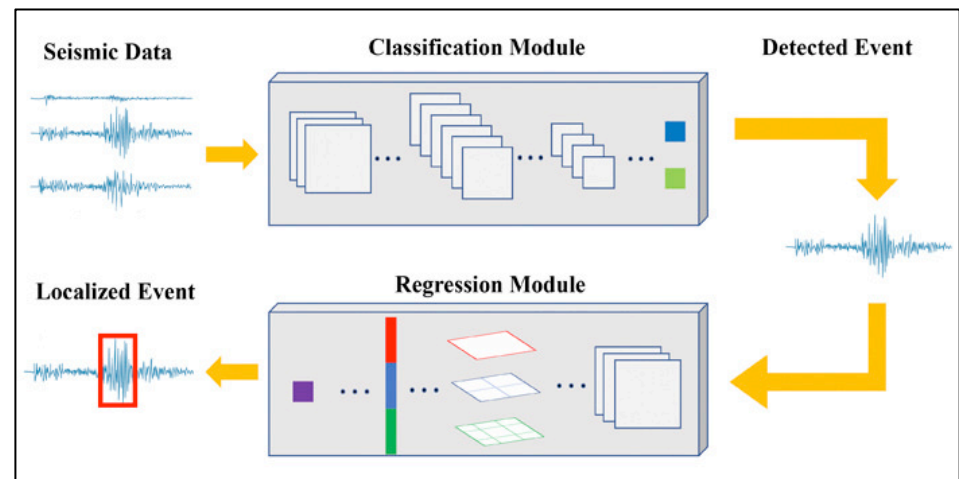


Shown here is part of the Los Alamos Neutron Science Center (LANSCE) magnet array, with the vacuum vessel end cap removed for magnetic field mapping, performed by Tennessee Technological University physics student Keegan Hoffman.

The mean neutron lifetime helps scientists predict the atomic makeup of the early universe and search for physics beyond the Standard Model of particle physics

Scientists have applied a 'deep dense neural network' approach to the detection of seismic events

- The LANL method identifies events of interest, earthquake signals, from 1-D time series data in a supervised manner (*IEEE Transactions on Geoscience and Remote Sensing* 2018)
 - The DeepDetect neural network design is based on a programming approach mimicking biological pathways in an animal brain, rather than providing the computer with step-by-step instructions to solve a problem
- The Lab is applying this technique to subsurface applications, e.g.:
 - Detection of leakage from carbon sequestration sites
 - Detection of induced seismicity caused by fluid injection practices



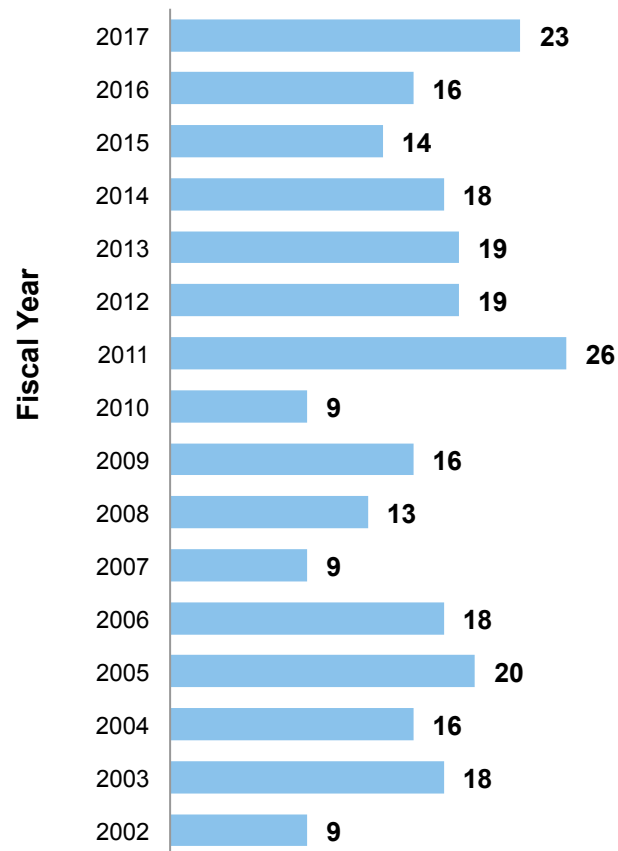
DeepDetect could be adapted to other domains or applications that involve monitoring routinely collected data, such as surveillance, scientific discovery, and data cleaning

Sustained Performance:

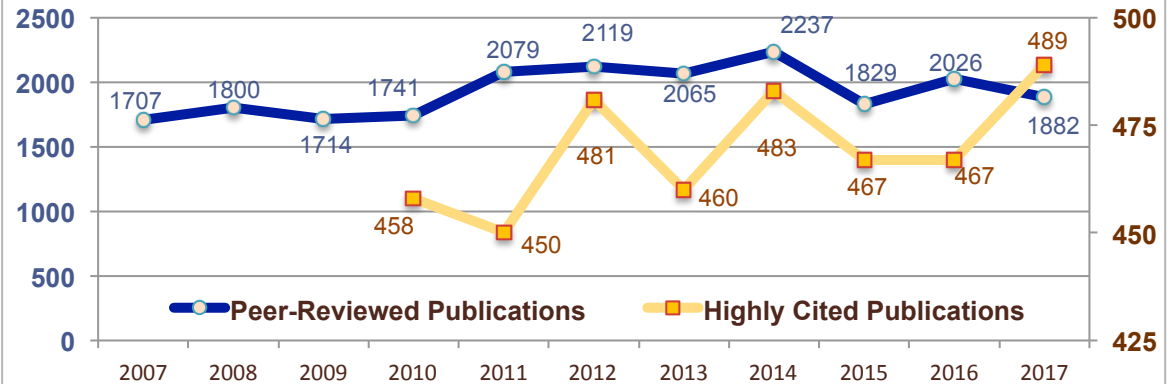
External recognition essential for recruiting, partnering...
and national security

Number of Awards/Fellows

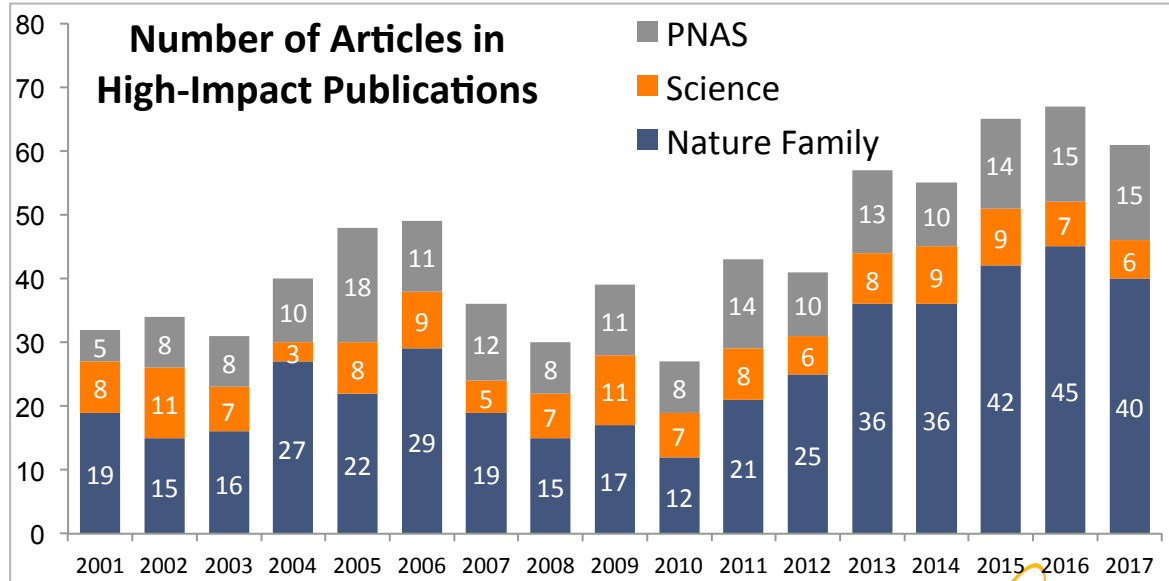
NAE, NAS, E.O. Lawrence, AAAS, APS, ACS,
PECASE, R&D 100, AGU, ASA, IEEE



Lab Publication Trends

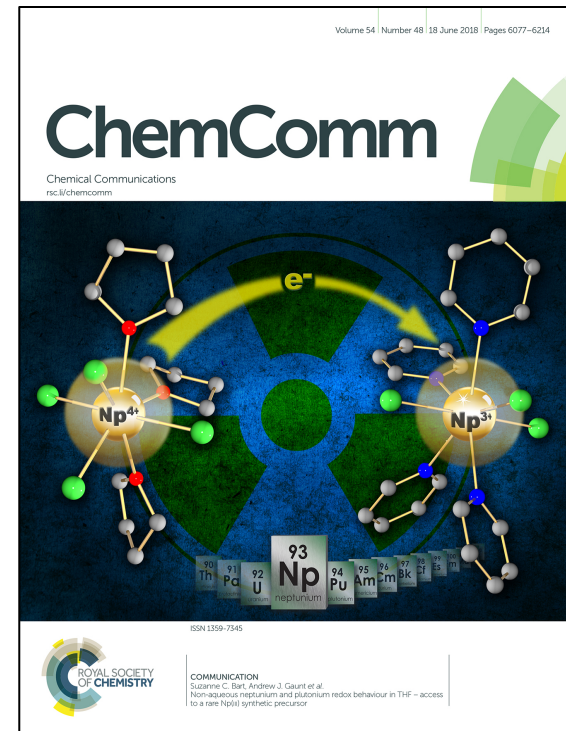


Number of Articles in High-Impact Publications



Researchers isolate new neptunium (III) compound

- Los Alamos and Purdue University researchers isolated and structurally characterized a new, rare, easily prepared, neptunium (III) [Np³⁺] starting material (***Chemical Communications* 2018**)
 - Most neptunium (III) is formed in nuclear reactors and contributes to the radiotoxicity of nuclear waste
 - Helps solve the problem of Np metal scarcity for research by converting readily accessible Np oxide/aqueous solutions to a non-aqueous Np(III) molecule
 - Enables comparison to uranium (III) and plutonium (III) chemistry



The **ChemComm** journal cover in June 2018 featured the Np(III) research.

The work helps elucidate new understanding of redox chemistry and makes Np(III) chemistry more accessible

Innovative 'lighthouse' radiation detectors quickly pinpoint radiation sources

- Small radiation detectors pinpoint radiation source in seconds, precisely determining the location, amount, and movement of a radioactive source, even in the presence of background radiation
 - New design transforms traditional omnidirectional detectors into directional detectors
 - Patented by the Lab and commercialized by industrial partners
- Technology grew out of Lab's 75 years of radiation detector experience
- LANL uses detectors on HAZMAT robots for emergency response and to conduct geologic surveys

Detectors reduce radiation exposure for workers and open up new areas for robotic monitoring to avoid potential hazards



Acoustic collimated beam (ACCObeam) provides precise, inexpensive monitoring of fractured rock, concrete, metal

- ACCObeam images objects using sound waves that are both low frequency and almost perfectly parallel (*Wave Motion* 2018)

- Simple piezoelectric disc in a hard plastic tube converts an electrical signal to sound waves
- Produces a highly collimated, powerful sound beam that also minimizes unwanted side lobes
- Can be used in almost any medium: mud, water, bone, rock, and metal
- In oil and gas wellbores, can penetrate beyond steel casing and wellbore cement to image 2–3 meters of surrounding rock without compromising image resolution



The ACCObeam technology builds on almost 30 years of Los Alamos research experience, resulting in four previous R&D 100 awards, a dozen U.S. and European patents, and numerous publications.



This technology is garnering interest in areas of subsurface energy and high explosives threat evaluation

Long-range wireless sensor network offers affordable, easy-to-use remote data collection

- Lab scientists and West Virginia Univ. developed a self-forming, self-healing, low-power sensor network, called the Long-range Wireless Sensor Network
 - This patented sensor network collects, processes, and transmits data in harsh environments anywhere on the globe
 - Low-power nodes transmit with long-range radio frequency or satellite communication
 - Nodes discover their own routes to the master node, routing around failed or removed nodes
- Grew out of LANL's decades of experience in developing ruggedized satellite components

Applications range from environmental assessment, agricultural and ranching uses, nonproliferation, and oil and gas exploration

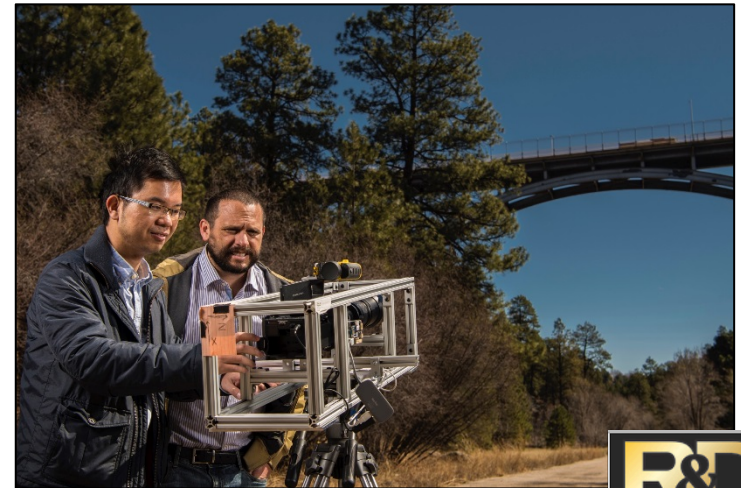


The nodes in this network are solar-powered and communicate via radio frequency.



ViDeoMAgic technology characterizes structural dynamic behavior, assesses structural and material health

- Los Alamos engineers developed method to extract pixel-level vibration and dynamics information from vibrating structures (***Journal of Intelligent Material System and Structures 2018***)
- ViDeoMAgic can assess health of civil, mechanical, and aerospace structures materials for damage, defects
 - Takes digital videos of vibrating structures and extracts high-spatial-resolution vibration/dynamics information
 - Patented technology works automatically, using unsupervised machine learning



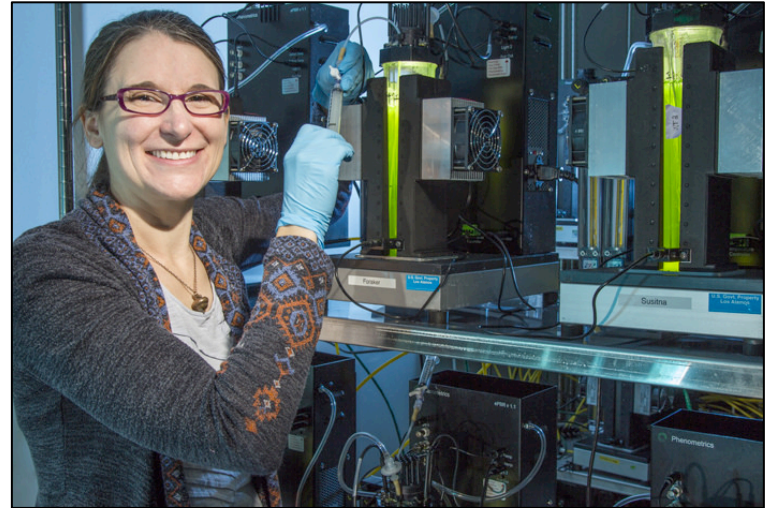
ViDeoMAgic (Video-Based Dynamic Measurement & Analysis) functions in non-ideal, real-world application environments



Such enhanced detection enables users to better identify incipient damage before it reaches a critical level of costly repairs, delays, or even deaths

Los Alamos study boosts algae's potential value as a biofuel

- LANL researchers and collaborators published the first report of a freshwater microalgae strain that uses raw plants as a carbon energy source (*Algal Research* 2018)
 - Study identified algae strains that can use plant substrates, such as switchgrass and corn stover (the part of the plant left in a field after harvest) to grow faster and produce more energy-rich lipids
- Results suggest that waste plant material could be used to increase the productivity of algae during cultivation for biofuels or bioproducts



Amanda Barry of Los Alamos's Bioenergy and Biome Sciences group and lead author on the study

Algae hold great potential as a renewable energy source because of their ability to produce refinery-compatible diesel and jet fuel precursors

Los Alamos chemists, computer modelers team up to unravel complex mechanical/chemical processes in explosive initiation

- Using computer modeling and a novel molecule design technique, Los Alamos scientists have replaced one “arm” of an explosive molecule to help unravel the first steps in the detonation process (***Chemical Science* 2018**)
 - The goal is to better understand an explosive’s sensitivity — and to ultimately make explosives safer for handling and storage
 - Using this method, researchers changed the sensitivity of common PETN-type explosives

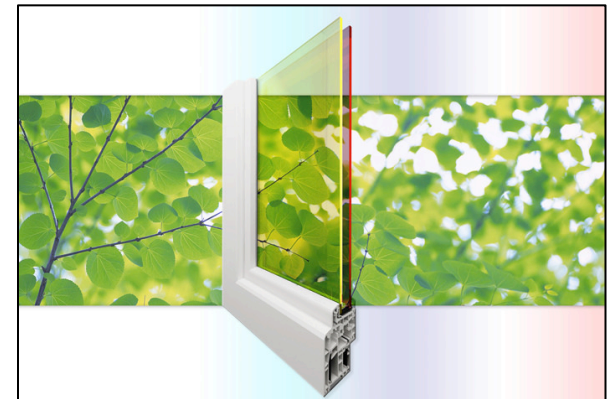


Los Alamos researchers Daniel Preston (left), Virginia Manner (center) and Geoff Brown prepare a drop-weight impact test on an explosive PETN derivative.

Method could guide the development of new explosives with tailored properties for specific applications

Using quantum dots, Lab researchers are creating double-pane solar windows that generate electricity with greater efficiency

- The double-pane windows use a new window architecture, layered with quantum dots, that turns windows into electric generators (*Nature Photonics* 2018)
 - Uses two different layers of low-cost quantum dots tuned to absorb different parts of the solar spectrum; solar cells integrated into the window frame collect the light and convert it to electricity
 - The key to this advance is “solar-spectrum splitting,” which processes separate higher- and lower-energy solar photons
- The approach complements existing photovoltaic technology by
 - adding high-efficiency sunlight collectors to existing solar panels, or
 - integrating them as semi-transparent windows into a building’s architecture

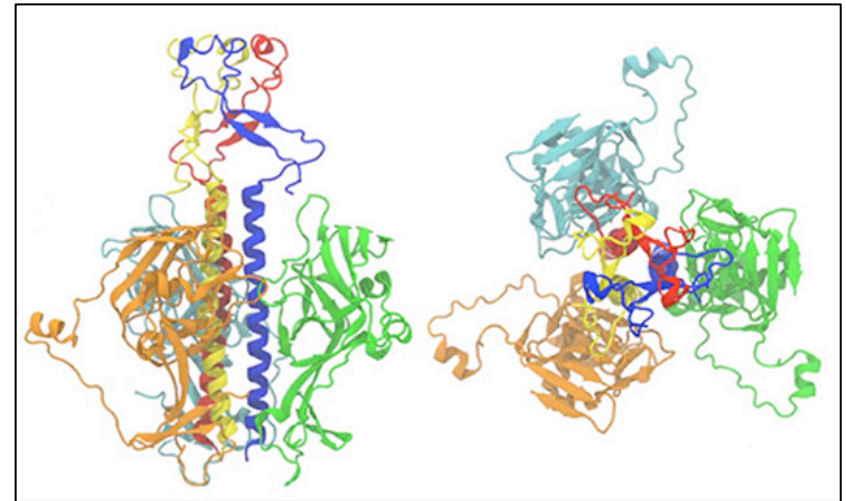


Window design would also create shading and insulation

Engineered quantum dots could bring down the cost of solar electricity and revolutionize the way we generate electricity

Los Alamos computer models provide valuable insight on how Ebola and Zika viruses infiltrate a host cell

- A LANL team used a Los Alamos-developed computational approach to generate, for the first time, atomic-level models of how Ebola and Zika proteins change their physical structure in order to enter a host cell (*Biomolecules* 2018)
 - The team then used the structure to explain how four antibodies can fight the infection and block the virus from entering the cell
- With this understanding, the team determined how antibodies take a multilevel approach to block viral entry and fight infection



A molecular dynamics computer model of the side view (left) and top view of the Ebola Virus structure that allows it to fuse with a cell.

The modeling capabilities provide an essential step toward vaccine and therapeutic medicine development